BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE (BITS) PILANI – Pilani Campus

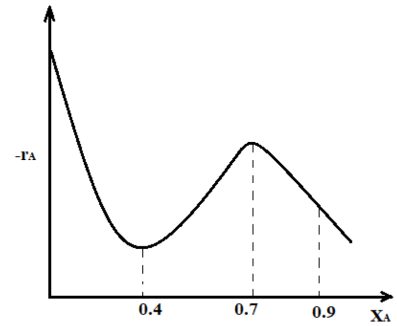
Title: **K**inetics and **R**eactor **D**esign (CHE F311)- End-Semester Examination (2023-24)

Date: 15.12.2023 Max.Marks: 120

PART- A: *Write final answers only.* **30 x 2 = 60 M**

S.No	***Question***
1.	The conversion for a second order, irreversible reaction (constant volume) $A \rightarrow B,$ in batch mode is given by ___
2.	The following half-life data are available for the irreversible liquid phase reaction, $A \rightarrow products$. The overall order of the reaction is________ Initial concentration (kmol/ m^3) | Half-life (min) 2 | 2 8 | 1
3.	An irreversible, homogeneous reaction A → Products, has the rate expression: $-r_A = \frac{2C_A^2+0.1\ C_A}{1+50\ C_A}$. where C_A is the concentration of A and C_A varies in the range 0.5-50 mol/m^3.For very high concentration of A, the reaction order tends to:_________
4.	A pollutant *P* degrades according to first-order kinetics. An aqueous stream containing *P* at 2 kmol/m^3 and volumetric flow the 1 m^3 /h requires a mixed flow reactor of volume V to bring down the pollutant level to 0.5 kmol/m^3 . The inlet concentration of the pollutant is now doubled and the volumetric flow rate is tripled. If the pollutant level is to be brought down to the same level of 0.5 kmol/m^3 , the volume of the mixed flow reactor should be increased by a factor of ___________
5.	The following **gas phase** reaction takes place in a continuous flow reactor, $A + 0.5\ B \rightarrow C$. A stoichiometric mixture of A and B at 300 K is fed to the rector. At 1 m along the length of the reactor, the temperature is 360 K. The pressure drop is negligible, and an ideal gas behavior can be assumed. Write the expression relating the concentration of A and B (C_A& C_B) in terms of limiting reactant A and conversion X_A
6.	The liquid phase reaction A→ Products is governed by the kinetics,$-r_A = kC_A^{0.5}$, if the reaction undergoes 75% conversion of A in 10 min in an isothermal batch reactor, the time (in min) for complete conversion of A is________

7. A liquid phase reaction is to be carried out under isothermal conditions. The reaction as a function of conversion has been determined experimentally and is shown in figure below. What choice of reactor of combination of reactors will require the minimum overall reactor volume, if a conversion of 0.9 is desired?

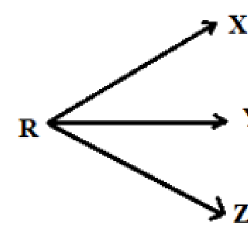


(A) CSTR followed by a PFR
(B) PFR followed by a CSTR
(C) CSTR followed by a PFR followed by CSTR
(D) PFR followed by a CSTR followed by a PFR

8. The liquid phase reaction A → products is carried out at constant temperature in a CSTR+ PFR) and gives a overall conversion of 95%. The CSTR has a volume of 75 L. Pure A is fed to the CSTR at a concentration C_{A0} =2mol/L and a volumetric flow rate of 4 L/min. The kinetics of the reaction given by $-r_A = 0.5\, C_A^2$. The conversion achieved by the CSTR is ________

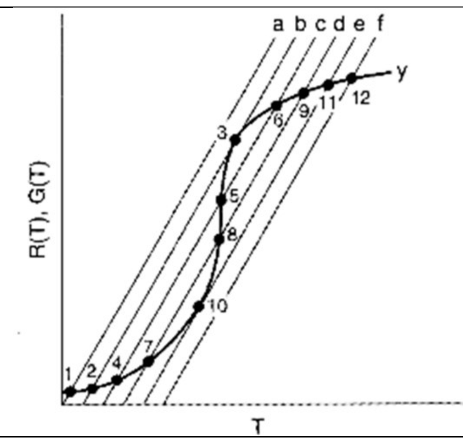
9. In the above arrangement, The volume of the PFR required (in liter) is ____

10. Reactant R forms three products X, Y, and Z irreversibly, as shown figure. The reaction rates are given by $r_x = k_1 C_R, r_y = k_2 C_R^{1.5}, r_z = k_3 C_R$. The activation energies for the formation of X. Y and Z are 40, 40 and 5 kJ/mol, respectively. The pre-exponential factors for all reactions are nearly the same. The desired conditions for maximizing the yield of X are _________



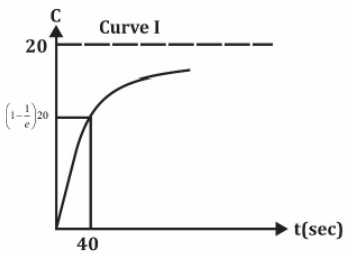
(A) high temperature, high concentration of R
(B) low temperature, low concentration of R
(C) low temperature, high concentration of R
(D) high temperature, low concentration of R

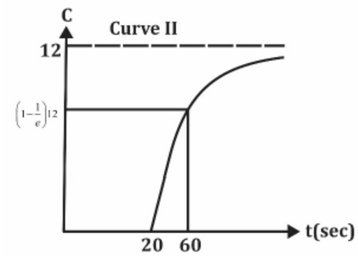
11. Develop ignition and extinction cure from the figure. Indicate the points clearly (numbers) with legends of X- & Y axis.



12. A step input tracer test is used to explore fluid flow patterns through a vessel of total volume equal to 1 m^3 /min. Identify a suitable flow model from the list given under Group II for each curve in Group I.

Group 1	Group 2
P. Curve 1	**1.** PFR and CSTR in series
Q. Curve 2	**2.** CSTR with dead space
	3. PFR in series with a CSTR and dead space
	4. CSTR





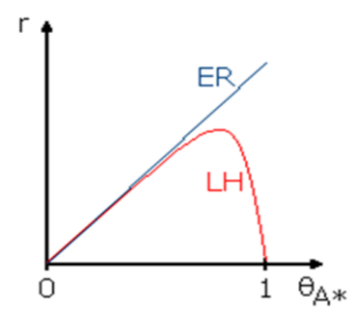
(A) P-4, Q-3 (B) P-4, Q-1 (C) P-2, Q-3 (D) P-2, Q-1 (NIGQ5)

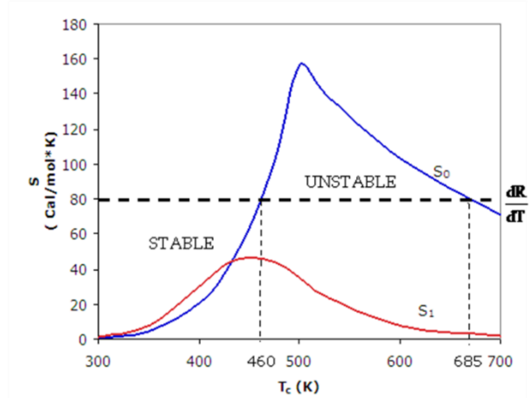
13. Define the Peclet number and Pectlet number for a real reactor is _____

14. Write down the steps involved in heterogeneous catalytic reactions.

15. Draw the concentration profiles (on a single plot) inside the spherical catalyst (R ; radius) having Φ= 0.01, 10 and 100 (C_A/C_{AS} vs r/R) for a first-order system. Assume external resistances are negligible.

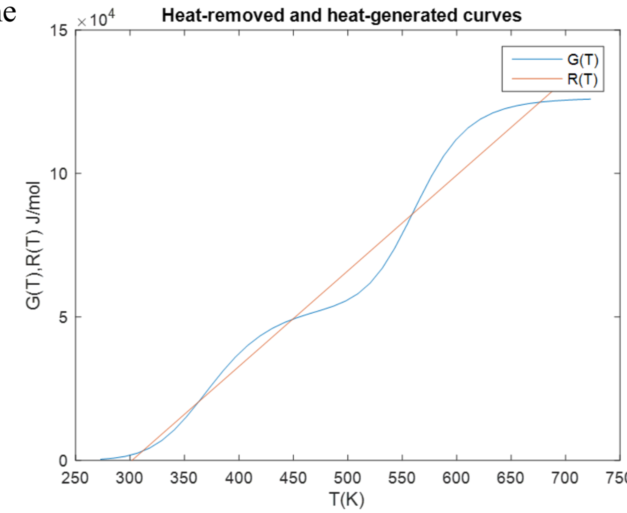
16. Write the two equations (in terms of adiabatic parameter (*k*), c_{po}, *E*, *T*, *etc* ...) to avoid runaway reactions in an ideal CSTR.

17.	Write down the chemical reactions occurring on a three-way catalyst for an engine exhaust.
18.	An impulse tracer input has been given separately for an ideal PFR, ten ideal CSTRs in series, and one ideal CSTR. Draw the corresponding *E(t) versus time* responses on a single plot. Mark the type of reactors in the plot.
19.	*ER*: Eley Rideal, *LH*: Langmuir. θ_A: fractional coverage, r: rate. Why *ER* > *LH* at high θ_A? assume the overall reaction is A+ B= C 
20.	Is it possible to eliminate the internal resistances completely for a heterogeneous catalytic reaction? If Yes/ No. and write the expression to check the internal resistances.
21.	Define *closed-closed* and *open-open vessel* boundary conditions for one-parameter model.

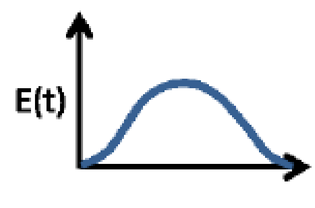
22.	Draw a schematic of the radial flow-packed bed reactor. Indicate the flow directions and advantages over other configurations.
23.	The overall rates of an isothermal catalytic reaction using spherical catalyst particles of diameter 1mm and 2 mm are r_{A1} and r_{A2} (in mol/(kg catalyst- h), respectively. The other physical properties of the catalyst particles are identical. If pore diffusion resistance is very high, the ratio r_{A2}/ r_{A1} is_______
24.	Write the residence distribution expression for a series of combinations of CSTR-PFR and PFR-CSTR ideal reactors (where τs is the space-time of the CSTR, and τp is the space-time of the PFR). Additionally, comment on the conversions when a first-order & other than first order reactions occurs in these combinations.
25.	What are the inferences from the following plot? (S_0 and S_1 are stabilities of zero and first-order reactions) 
26.	Find the first-order rate constant for the disappearance of A in the gas reaction $2A \rightarrow R$ if, on holding the pressure constant, the volume of the reaction mixture, starting with 80% A, decreases by 20% in 3 min.

27. How much does a reaction rate with an activation energy of 15,000 Cal/mole vary when the temperature is increased from 300 to 400 K?

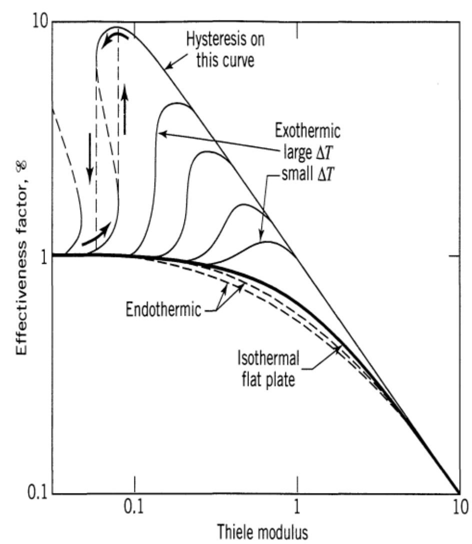
28. Identify stable and unstable points on the curve.



29. Draw a schematic model for complete macro mixing in a tubular reactor based on the figure.



30. What are the parameters required to generate this plot? Why is it happening for exothermic reactions only?



PART B **6 x 10= 60 M**

Note: *Make the appropriate assumptions by clearly stating them, if necessary*

1. An elementary liquid phase reaction $P \Leftrightarrow Q$ is carried out in an ideal flow reactor. The rate of consumption of P is given by $-r_P = C_p - 0.5\, C_Q$. The feed contains only the reactant P at a concentration of 1 mol lit^{-1}. Calculate the space-time/ time required to achieve *75% of the equilibrium conversion* for a) PFR, b) CSTR, c) batch reactor.

2. Normal butane, C_4H_{10}, is to be isomerized to iso- butene in a plug-flow reactor ($n - C_4H_{10} \leftrightarrow i - C_4H_{10}$) Isobutane is a valuable product that is used in the manufacture of gasoline additives. The reaction is to be carried out adiabatically in the liquid phase under high pressure using essentially trace amounts of a liquid catalyst which gives a specific reaction rate of 31.1 h^{-1} at 360 K. Calculate the PFR volume necessary to process 163 kmol/h at 70% conversion of a mixture 90 mol % n-butane and 10 mol% i-pentane, which is considered an inert. The feed enters at 330 K. (Hint: Levenspiel plot may be useful)

   Data: ΔH_{RX}= - 6900 J/mol-butane, E= 65700 J/mol, K_C= 3.03 at 60 ºC, C_{AO}= 9.3 kmol/dm^3, R= 8.31 J/mol. K

   Specific heats: n-butane: 141, i-butane: 141, i-pentane= 161 J/mol-K.

   This equation may be useful:

$$X = \frac{\sum \Theta_i \widetilde{C}_{Pi}(T - T_{i0})}{-\left[\Delta H^o_{Rx}(T_R) + \Delta \hat{C}_P (T - T_R)\right]}$$

3. Consider the overall reaction $A + B \Leftrightarrow C$. A possible catalyst material contains two different types of reactive sites, X and Y. Both A and B adsorb on X and Y, but the reaction proceeds only if *A* adsorbs on *X* and *B* on *Y*. The following mechanism describes this reaction:

$$A + X = A.X \qquad (1)$$

$$A + Y = A.Y \qquad (2)$$

$$B + X = B.X \qquad (3)$$

$$B + Y = B.Y \qquad (4)$$

$$A.X + B.Y \rightarrow C + X + Y \quad (5)$$

   a. What is the production rate of C if Reaction 5 is irreversible and Reactions 1–4 reach equilibrium? Hint: you can assume you know the monolayer coverage amounts of both the X and Y available sites. Total free sites available at time zero are C_{TX}, C_{TY}.

   b. If the equilibrium constants for Reactions 1–4 are of the same order of magnitude, what happens to the production rate of C if very large or very small ratios of A to B are feed to the reactor?
   (Hint: $C_{Tx}= C_{A.X}+ C_{B.X}+ C_{SX}$, $C_{TY}=C_{A.Y}+C_{B.Y}+C_{SY}$, where C_{tx} total site balance of X, Csx is the vacant sites in X)

4. A specific spherical porous catalyst with a pellet diameter of l/8 in. has a Thiele modulus of 0.5 for a first-order reaction and gives 90% conversion in a packed bed reactor. It is proposed to replace this catalyst by the exact same catalyst but with pellets of l/4 or l/2 in. to reduce the pressure drop? How will the conversion change with these catalysts? [Hint: $\Phi = R\sqrt{\frac{k_1^{11} S_a \rho_c}{De}}$ and $\eta = \frac{rate_{Obs}}{rate_{intrinsic}}$]

5. A first order reaction $A \rightarrow B$ is carried out in a 10 cm dia tubular reactor with 6.36 m in length. k= 0.25min^{-1}. The results of the tracer test carried out on this reactor are provided.

t(min)	0	1	2	3	4	5	6	7	8	9	10	12	14
C(mg/L)	0	1	5	8	10	8	6	4	3	2.2	1.5	0.6	0

Calculate the conversion i) closed vessel dispersion model; ii) PFR; iii) Single CSTR; iv) Tanks in series

$$X = 1 - \frac{4q \exp(\mathrm{Pe}_r/2)}{(1+q)^2 \exp(\mathrm{Pe}_r q/2) - (1-q)^2 \exp(-\mathrm{Pe}_r q/2)} \quad \text{where } q = \sqrt{1 + 4\mathbf{Da}/\mathrm{Pe}_r}$$

6. Consider the aqueous reactions

$$A + B \xrightarrow{k_1} R, \text{ desired} \qquad \frac{dC_R}{dt} = 1.0\, C_A^{1.5}\, C_B^{0.3}, \text{ mol/liter·min}$$

$$A + B \xrightarrow{k_2} S, \text{ unwanted} \qquad \frac{dC_S}{dt} = 1.0\, C_A^{0.5}\, C_B^{1.8}, \text{ mol/liter·min}$$

For 90% conversion of A find the concentration of R in the product stream. Equal volumetric flow rates of the A and B streams are fed to the reactor, and each stream has a concentration of 20 mol/liter of reactant. The flow in the reactor follows.

(a) Plug flow

(b) Mixed flow

(c) Plug flow with side entries of B

ALL THE BEST